

Quantum corrections to the thermodynamic potential of interacting Bosons in a trap

Subhasis Sinha

The Institute of Mathematical Sciences, Madras 600 113, India.

(February 1, 2008)

We calculate the quantum corrections of the thermodynamic quantities of a system of confined Bosons at finite temperature. Systematically quantum corrections are written in a series of \hbar , which is convergent when kT is much larger than the spacing between energy levels of the system. We apply this method to calculate analytically the thermodynamic potential of a weakly interacting Bose-gas confined in 3-d harmonic oscillator potential. For large number of particles, quantum corrections become small, and contribute to the finite size corrections to scaling.

PACS numbers:03.75.Fi,32.80.Pj

There has been renewed interest in the Bose-Einstein condensation(BEC) after its experimental demonstration by Anderson et al [1]. It has now become possible to measure the relevant thermodynamic quantities of a system of weakly interacting Bosons in a magnetic trap [2,3]. In these experiments, the temperature dependence of the condensate fraction and the release energy are measured. Theoretically, the thermodynamic properties of homogeneous Bose gas was studied by several authors starting from London [4]. The thermodynamic properties of the inhomogeneous Bose gas was studied by Legget et al [5,6]. After the recent experimental developments, there is a new impetus to understand the thermodynamic properties of interacting inhomogeneous Bose gas. Within the local density approximation(LDA), Stringari et al [7] have calculated the thermodynamic quantities numerically and shown scaling properties of strongly interacting bosons in a trap and since then several calculations have been reported by various authors [8,9]. In these papers the thermodynamic properties of inhomogeneous gas has been calculated within the LDA, neglecting the quantum corrections which may be important.

In this paper we develop a systematic semiclassical \hbar -expansion for thermodynamic quantities of an interacting bose gas which takes into account the quantum corrections. We follow a method analogous to the extended Thomas-Fermi method(ETF) which has been successfully applied in the case of finite fermion systems, like nuclei, atoms, clusters etc. It is well known that the semiclassical expansion of the smooth part of the quantum density of states can be expanded in powers of \hbar . The leading term in this expansion is the Thomas-Fermi level density. Systematic \hbar corrections to the leading approximation may then be obtained using the well known Wigner-Kirkwood(WK) expansion [10]. In the case of finite fermion systems this is what is usually referred to as the extended Thomas-Fermi approximation [11].

We first develop a systematic \hbar expansion using the W-K method [10]. Consider the single particle Hamiltonian H for a system of particles, which satisfies the equation,

$$H\psi_n = E_n\psi_n \quad (1)$$

where E_n are eigenvalues and ψ_n are corresponding wave functions. The canonical partition function of the system

is defined as

$$Z_0(\beta) = \sum_n e^{-\beta E_n}, \quad (2)$$

where β is, for our purposes, a parameter with the dimension of inverse energy. We first briefly review the method as applied to the finite fermion system [11]. To extract thermodynamic quantities of the finite fermion system from the canonical partition function, a weight function is defined as $w_F = \frac{\pi\beta T}{\sin(\pi\beta T)}$. By using this weight function one can write the grand potential of the system in the following way,

$$kTq(T, z) = \mu N - E + TS \\ = L_\mu^{-1} \left[\frac{Z_0(\beta)w_F}{\beta^2} \right]. \quad (3)$$

In integral representation,

$$kTq(T, z) = \frac{1}{2\pi i} \int_{\epsilon-i\infty}^{\epsilon+i\infty} e^{\beta\mu} \frac{Z_0(\beta)w_F}{\beta^2} d\beta \quad (4)$$

where the contour is closed from left, enclosing all the negative poles. Summing all residues we obtain the known result [12],

$$q(T, z) = \sum_n (1 + ze^{-E_n/kT}), \quad (5)$$

where $z = e^{\beta\mu}$ is the fugacity. We may extend this method to Bosons also, by taking a suitable weight function,

$$w_B = \frac{-\cos(\pi\beta T)\pi\beta T}{\sin(\pi\beta T)}. \quad (6)$$

The grand potential of an ensemble of bosons can be written in terms of the following integral,

$$kTq(T, z) = \frac{1}{2\pi i} \int_{\eta-i\infty}^{\eta+i\infty} e^{\beta\mu} \frac{Z_0(\beta)w_B}{\beta^2} d\beta. \quad (7)$$

The line of integration is chosen in such a way that all the positive poles(excluding zero) are to the right side

of the line. Since the chemical potential $\mu < E_n$ for bosons, we close the contour from right, and summing all the residues at the positive poles inside the contour, we obtain the well known result [12],

$$q(z, T) = - \sum_n \log(1 - ze^{-E_n/kT}). \quad (8)$$

From the above thermodynamic potential we can calculate all thermodynamic quantities.

To do a systematic \hbar expansion of Bosons, we start from high temperature limit. Neglecting zero point energy and the occupation number of ground state, we can do W-K expansion of canonical partition function. For the semiclassical expansion of the partition function, it is most convenient to take plane wave basis for calculation of the canonical partition function.

$$Z_0(\beta) = \frac{1}{h^3} \int d^3p \int d^3r e^{-i\vec{p}\cdot\vec{r}/\hbar} e^{-\beta H} e^{i\vec{p}\cdot\vec{r}/\hbar} \quad (9)$$

To evaluate the partition function, we write,

$$\begin{aligned} u(\vec{r}, \vec{p}, \beta) &= e^{-\beta H} e^{i\vec{r}\cdot\vec{p}/\hbar} \\ &= e^{-\beta H_{cl}} e^{i\vec{r}\cdot\vec{p}/\hbar} w(\vec{r}, \vec{p}, \beta), \end{aligned} \quad (10)$$

where H_{cl} is the classical hamiltonian $H_{cl} = \frac{p^2}{2M} + V(\vec{r})$ and u obeys the Bloch equation,

$$\frac{\partial u}{\partial \beta} + Hu = 0 \quad (11)$$

with the boundary condition

$$\lim_{\beta \rightarrow \infty} u = e^{i\vec{p}\cdot\vec{r}/\hbar}. \quad (12)$$

Substituting u in the above equation, we obtain the following equation for w .

$$\begin{aligned} \frac{\partial w}{\partial \beta} &= -i\hbar \left[\frac{\beta}{M} (\vec{p} \cdot \nabla V) w - \frac{1}{M} (\vec{p} \cdot \nabla V) \right] + \\ &\frac{\hbar^2}{2M} [\beta^2 (\nabla V)^2 w - \beta (\nabla^2 V) w + \nabla^2 w - 2\beta (\nabla V \cdot \nabla w)] \end{aligned} \quad (13)$$

The above equation can be solved order by order in \hbar , by expanding w as a power series in \hbar .

$$w = 1 + \hbar w_1 + \hbar^2 w_2 + \dots \quad (14)$$

Upto the order \hbar^2 , canonical partition may then be written as [11],

$$\begin{aligned} Z_{wk}(\beta) &= \frac{1}{(2\pi\hbar)^3} \int d^3p e^{-\beta \frac{p^2}{2M}} \int d^3r e^{-\beta V(\vec{r})} \\ &\times \left[1 - \frac{\beta^2 \hbar^2}{24M} \nabla^2 V(\vec{r}) \right], \end{aligned} \quad (15)$$

where $V(r)$ is the effective single particle potential. Inserting this expression for canonical partition function in

equation (7), we obtain the grand potential of the normal state.

$$\begin{aligned} q(z, T) &= - \frac{1}{(2\pi\hbar)^3} \int d^3p \int d^3r [\log(1 - ze^{-\beta(\frac{p^2}{2M} + V(\vec{r}))}) \\ &- \frac{\hbar^2}{24M} \nabla^2 V(\vec{r}) \frac{\partial^2}{\partial \mu^2} \log(1 - ze^{-\beta(\frac{p^2}{2M} + V(\vec{r}))})] \end{aligned} \quad (16)$$

After doing the p integration we get the following form of the density of the grand potential upto order \hbar^2 .

$$F(\vec{r}) = \frac{1}{\lambda^3} [g_{5/2}(\tilde{z}) - \frac{\hbar^2}{24M} \nabla^2 V(\vec{r}) \frac{\partial^2}{\partial \mu^2} g_{5/2}(\tilde{z})] \quad (17)$$

where the $g_n(x)$ and λ are defined as,

$$\lambda = \frac{2\pi\hbar}{\sqrt{2\pi M kT}}; \quad g_n(x) = \sum_{i=1}^{\infty} \frac{x^i}{i^n}. \quad (18)$$

and the effective fugacity is $\tilde{z} = ze^{-\beta V(\vec{r})}$.

To check the correctness of the above formalism, we first apply it to a system of bosons in 3-d isotropic harmonic oscillator(h.o) confinement. Following our method, grand potential of the normal state is given by,

$$q(z, T) = \left(\frac{kT}{\hbar\omega}\right)^3 [g_4(z) - \frac{1}{8}(\beta\hbar\omega)^2 g_2(z)] \quad (19)$$

From this grand potential we can derive the number of particles and the energy of the normal state.

$$\begin{aligned} N_e &= z \left(\frac{\partial q}{\partial z} \right)_T \\ &= \left(\frac{kT}{\hbar\omega} \right)^3 [g_3(z) - \frac{1}{8}(\beta\hbar\omega)^2 g_1(z)] \end{aligned} \quad (20)$$

$$\begin{aligned} U &= - \left(\frac{\partial q}{\partial \beta} \right)_z \\ &= kT \left(\frac{kT}{\hbar\omega} \right)^3 [3g_4(z) - \frac{1}{8}(\beta\hbar\omega)^2 g_2(z)] \end{aligned} \quad (21)$$

Above quantities may also be derived by using density of state of the system. Exact canonical partition function of the 3-d h.o is given by,

$$Z(\beta) = \frac{1}{[2 \sinh(\frac{\beta\hbar\omega}{2})]^3}. \quad (22)$$

Density of states can be calculated by taking inverse laplace transform of the canonical partition function with respect to β . Also the same results may be obtained by Euler-Maclaurin summation method [9]. From the above calculation we have seen that, thermodynamic quantities may be expanded in a series of a dimensionless parameter $\beta\hbar\omega$. This series will converge when $\beta\hbar\omega \leq 1$. However at low temperatures, $\beta\hbar\omega \approx 1$, and Wigner-Kirkwood expansion breaks down. At these temperature, only few low energy states are occupied, so energy levels can not be taken as continuous.

In the systems which show macroscopic occupation of ground state at finite temperature, chemical potential of the system tends to zero. As $z \rightarrow 1$, the higher order terms in \hbar expansion show infrared divergence. To regulate such divergences fugacity of the system can be replaced by $ze^{-\Delta E/kT}$, where ΔE is the natural energy gap of finite size systems [13]. This is equivalent to introducing a infrared momentum cutoff $\approx 1/L$, where L is the system size.

Having checked the formalism, we now apply above method to real physical situation that of a non ideal Bose gas. In recent experiment Ensher et al [2] measured the thermodynamic quantities of 40000 Rb^{87} atoms, for which s-wave scattering length is $\approx 100a_0$, where a_0 is Bohr radius.

Within Hartree-Fock theory of bosons, non-condensate part satisfies the following Schrödinger's equation [5],

$$[-\frac{\hbar^2}{2M}\nabla^2 + \frac{1}{2}M\omega^2 r^2 + 2u\rho(r)]\psi_i(r) = \epsilon_i\psi_i(r), \quad (23)$$

and the condensate part satisfies Gross-Pitaevskii equation,

$$[-\frac{\hbar^2}{2M}\nabla^2 + \frac{1}{2}M\omega^2 r^2 + 2u\rho_{nc}(r) + u\rho_c(r)]\phi(r) = \epsilon_0\phi(r), \quad (24)$$

where $\rho_{nc}(r)$ and $\rho_c(r)$ are the densities of non-condensate and condensate part, and $\rho = \rho_c + \rho_{nc}$. The interaction strength is given by, $u = \frac{4\pi\hbar^2 a}{M}$. Neglecting the kinetic energy of the condensate, the lowest energy eigenvalue may be approximated by,

$$\epsilon_0 \approx \frac{1}{2}\hbar\omega(15N_0\frac{a}{l})^{2/5} + 2u\rho_{nc}(0). \quad (25)$$

Further within the same approximation condensate density can be written as,

$$\rho_c(r) = \frac{1}{u}(\epsilon_1 - V(r)), \quad (26)$$

where $\epsilon_1 = \frac{1}{2}\hbar\omega(15N_0\frac{a}{l})^{2/5}$. The above approximation is valid for large number of condensate atoms N_0 and for strong repulsive interaction. This approximation breaks down within a small region near the critical temperature, where the number of condensate atoms become very small. For the non-condensate part we may use the formalism developed earlier. Using equation (17), the local thermodynamic potential of the non-condensate atoms can be written as,

$$F(r) = \frac{1}{\lambda^3}[g_{5/2}(\tilde{z}_{eff}) - \frac{\hbar^2}{24M}\nabla^2 V_{eff}g_{1/2}(\tilde{z}_{eff})], \quad (27)$$

where $\tilde{z}_{eff} = e^{\beta(\mu - V_{eff}(r))}$ and $V_{eff}(r) = V(r) + 2u\rho(r)$. For perturbative expansion we write the effective fugacity in the following form.

$$\tilde{z}_{eff} = \tilde{z} \exp[\beta(\epsilon_1 - V(r) - 2u\rho_c(r) + 2u(\rho_{nc}(0) - \rho_{nc}(r)))] \quad (28)$$

where, $\tilde{z} = e^{\beta(\mu - \epsilon_0)}$, which is always less than 1. Assuming weak coupling, we expand the functions in terms of $2u(\rho_{nc}(0) - \rho_{nc}(r))$. The perturbative expansion in this method turns out to be well behaved [8]. Excluding the non-condensate part, the effective fugacity can be written as,

$$\begin{aligned} \tilde{z}_{eff} &= \tilde{z}e^{\beta(V(r) - \epsilon_1)} \quad \text{for } r < r_0 \\ &= \tilde{z}e^{\beta(\epsilon_1 - V(r))} \quad \text{for } r > r_0, \end{aligned} \quad (29)$$

where r_0 is the turning point of Thomas-Fermi density ρ_c . From the above expression we can see there is no expansion parameter for condensate part. We approximate the local chemical potential within the condensate by its mean value. To calculate the free energy of the system within mean field theory, we subtract self energy from the total energy of the system. The self energy contribution is given by,

$$E_s = u \int \rho_{nc}^2(r) d^3r. \quad (30)$$

In the following calculation we replace the coupling by a dimensionless parameter $\eta = (\sqrt{\frac{2}{\pi}}\frac{a}{l}N^{1/6})^{2/5}$. Upto order $\eta^{5/2}$ and \hbar^2 the thermodynamic potential is given by,

$$\begin{aligned} q(z, T)/N &= t^3 \tilde{g}(4, \tilde{z}, 1/2, \alpha\eta\tilde{\beta}) + \\ &\frac{2}{\sqrt{\pi}}t^3 \sqrt{(\alpha\eta\tilde{\beta})}[g_{7/2}(\tilde{z}) + \frac{2}{3}\alpha\eta\tilde{\beta} g_{5/2}(\tilde{z}e^{-2/5\alpha\eta\tilde{\beta}})] \\ &+ 2\eta^{5/2}t^{7/2}[\zeta(3/2)g_3(\tilde{z}) - \frac{1}{2}F(3/2, 3/2, 3/2, \tilde{z})] \\ &- \frac{1}{8N^{2/3}}t[\tilde{g}(2, \tilde{z}, 1/2, \alpha\eta\tilde{\beta}) + \\ &\frac{2}{\sqrt{\pi}}\sqrt{(\alpha\eta\tilde{\beta})}[g_{3/2}(\tilde{z}) - \frac{2}{3}\alpha\eta\tilde{\beta}g_{1/2}(\tilde{z}e^{-2/5\alpha\eta\tilde{\beta}})] \\ &+ 2\eta^{5/2}t^{1/2}(\zeta(3/2)g_1(\tilde{z}) - F(1/2, -1/2, 5/2, \tilde{z}))], \end{aligned} \quad (31)$$

where the new functions and parameters are defined by,

$$\tilde{g}(s, x, t, y) = \sum_{i=1}^{\infty} \frac{x^i}{i^s} I(t, iy) \quad (32)$$

$$I(t, y) = \frac{1}{\sqrt{\pi}} \int_0^{\infty} dx e^{-x} (x + y)^{(t-1)} \quad (33)$$

$$F(\alpha, \beta, \gamma, x) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \frac{x^{(i+j)}}{i^{\alpha} j^{\beta} (i+j)^{\gamma}} \quad (34)$$

$$\alpha = \frac{1}{2}(15\sqrt{\frac{\pi}{2}}N_0/N)^{2/5} \quad (35)$$

$$t = 1/\tilde{\beta} = kT/(\hbar\omega N^{1/3}) \quad (36)$$

For small value of $\alpha\eta$, the function $\tilde{g}(s, \tilde{z}, 1/2, \alpha\eta\tilde{\beta})$ can be written as $g_s(\tilde{z})$. Condensate fraction can be calculated from the thermodynamic potential,

$$N_0/N = 1 - z \frac{\partial(q(z,T)/N)}{\partial z} \quad (37)$$

For $T < T_c$, $\tilde{z} \approx 1$. To regulate some divergent terms appearing in the \hbar^2 corrections, we set $\tilde{z} \approx e^{-\beta\hbar\omega}$, which is the natural energy gap from ground state. From the above expression we can see that the condensate fraction and other thermodynamic quantities are not fully scale invariant with respect to the dimensionless scaling parameters η and t . But the extra terms coming from the quantum corrections contain a factor $1/N^{2/3}$. These terms depend on the number of particles in the system, and give finite size corrections to the scaling form of the thermodynamic quantities. In the large N limit and also in the high temperature phase, quantum corrections are negligible. But for small quantum confined systems they give finite corrections to the free energy.

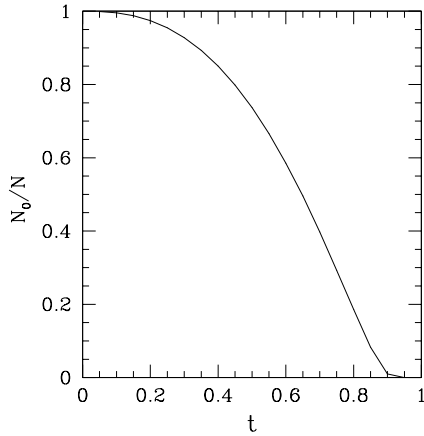


FIG. 1. Condensate Fraction for 10,000 atoms, $\eta=0.18$.

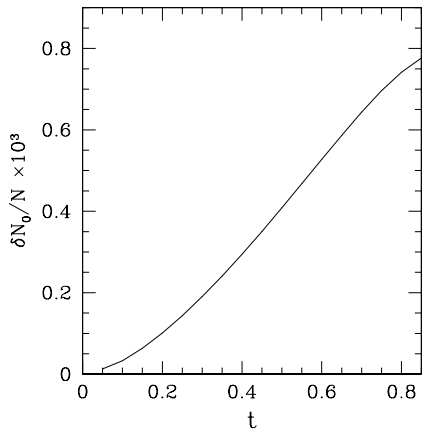


FIG. 2. Finite size correction to condensate fraction for 10,000 atoms, where t is reduced temperature.

For real physical systems the typical value of the parameter η which determines the two-body interaction strength varies from 0.1 – 0.25. In Fig.1 we have shown

the variation of condensate fraction with reduced temperature t , by choosing $N = 10,000$ atoms and the dimensionless parameter $\eta = 0.18$. In Fig.2 we have shown the finite size correction to the condensate fraction for same values of the parameters. From the graph we can see that the first order quantum correction is two order smaller than the leading order contribution.

In conclusion, we have developed an extended Thomas-Fermi method at finite temperature for a system of Bosons. Systematic quantum corrections may be written in a series of a dimensionless parameter $\beta\hbar\omega$, which converges for the temperatures larger than the average spacing between energy levels. We have applied our method to a system of weakly interacting Bose gas confined in isotropic harmonic oscillator potential. Thermodynamic potential and condensate fraction are calculated analytically upto $\eta^{5/2}$ and \hbar^2 order. Leading terms in \hbar are the functions of scaling parameters t and η only, but leading order quantum corrections give N dependent corrections to the scaling form. In present situation quantum corrections are negligibly small. But quantum corrections will be important for small number of particles and for low dimensional systems. Also its magnitude depends on the nature of confinement potential. This method may be applied to investigate the properties of a system of confined charged bosons in weak magnetic field.

I would like to thank M.V.N. Murthy and R.K. Bhaduri for helpful discussions.

-
- [1] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, *Science* **269**, 198 (1995).
 - [2] J. R. Ensher, D. S. Jin, M.R. Matthews, C.E. Weiman and E. A. Cornell, *Phys. Rev. Lett.* **77**, 416(1996).
 - [3] M. O. Mews, M.R. Andrews, N.J. van Druten, D.M. Kurn, D.S. Durfee, and W. Ketterle, *Phys. Rev. Lett.* **77**, 416(1996).
 - [4] F. London, *Nature* **141**, 643(1938) ; L. Landau, *J.phys. USSR* **5**, 71(1941).
 - [5] V. V. Goldman, I. F. Silvera and A. J. Leggett, *Phys. Rev.B* **24**, 2870(1981).
 - [6] J. Oliva, *Phys. Rev. B* **39**, 4197(1989).
 - [7] S.Giorgini, L. P. Pitaevskii, and S. Stringari, *Phys. Rev. Lett.* **78**, 3987(1996).
 - [8] H. Shi and W. M. Zheng, *Phys. Rev. A* **56**, 2984(1997).
 - [9] H. Haugerud, T. Haugset and F. Ravndal, *Phys. Lett. A* **225**, 18(1997).
 - [10] E. Wigner, *Phys. Rev.* **40**, 749(1932) ; J. G. Kirkwood, *Phys. Rev.* **44**, 31(1933).
 - [11] Matthias Brack and Rajat. K. Bhaduri, *Semiclassical Physics*, (Addison-Wesley publishing company, 1997).
 - [12] R. K. Pathria, *Statistical Mechanics*, (Pergamon Press, New York, 1972).
 - [13] R. Masut and W. J. Mullin, *Am. J. Phys.* **47**, 493(1979).